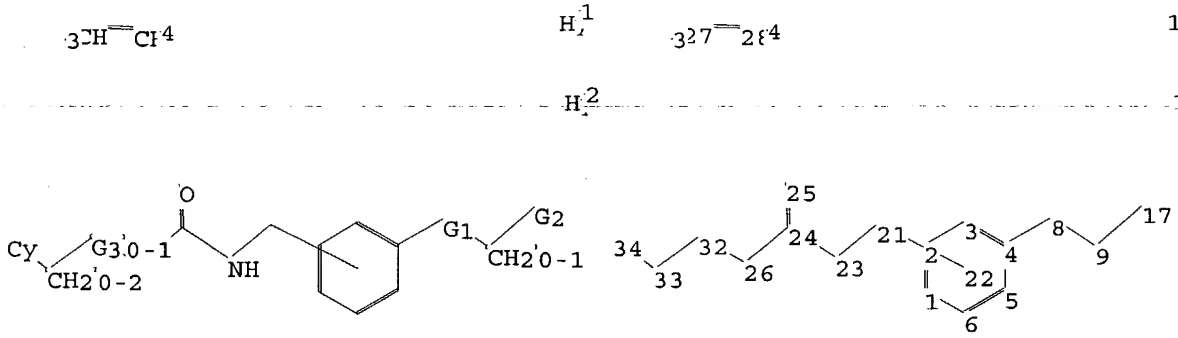
=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538.str



chain nodes :
8 9 10 11 17 21 23 24 25 26 27 28 32 33 34
ring nodes :
1 2 3 4 5 6
chain bonds :
4-8 8-9 9-17 21-23 23-24 24-25 24-26 26-32 27-28 32-33 33-34
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-8 8-9 9-17 21-23 23-24 24-25 26-32 32-33 33-34
exact bonds :
24-26 27-28
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:Atom 11:Atom
17:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 32:CLASS 33:CLASS 34:Atom
Generic attributes :
10:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System : Monocyclic
11:

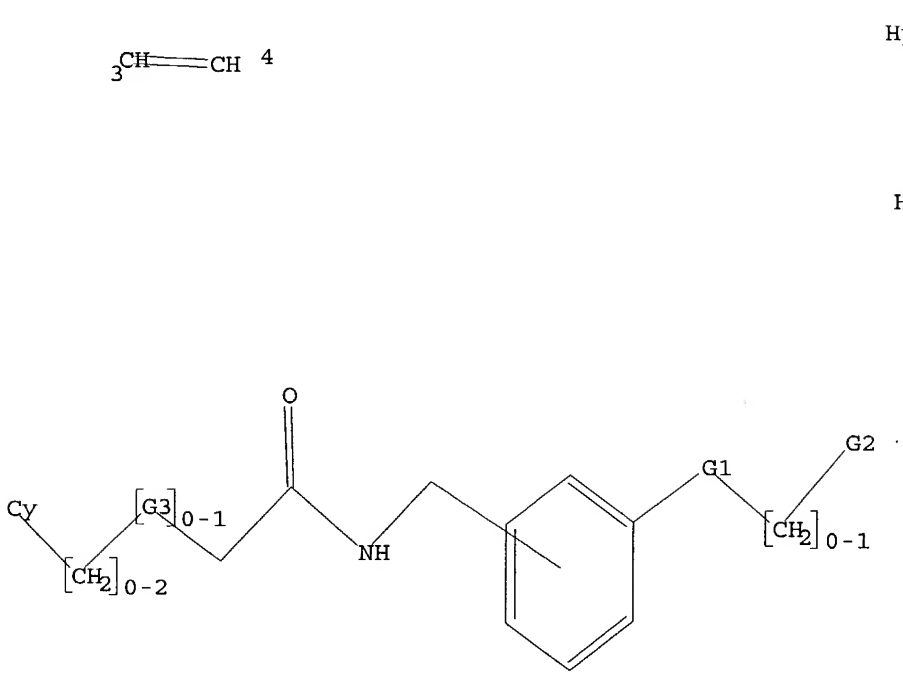
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System : Monocyclic

Element Count :
Node 10: Limited
C,C5
N,N1
S,S0
O,O0

Node 11: Limited
C,C4
N,N2
O,O0
S,S0

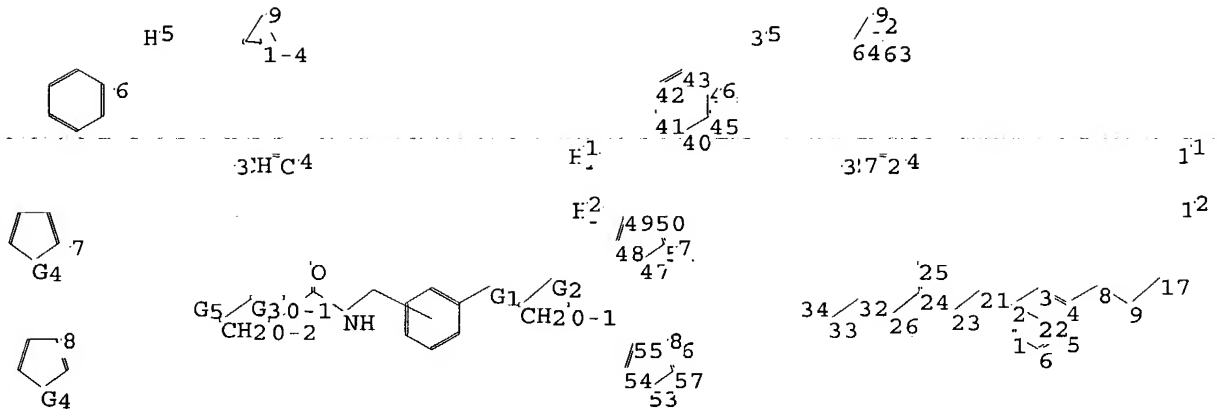
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,N
G2 [@1],[@2]
G3 CH2,[@3-@4]

```
Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 18:47:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 115414 TO ITERATE

  0.9% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0

L2             0 SEA SSS SAM L1

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1840

L3     SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L4     SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538 (a).str
```



chain nodes :
8 9 10 11 17 21 23 24 25 26 27 28 32 33 34 39
ring nodes :
1 2 3 4 5 6 40 41 42 43 44 45 47 48 49 50 51 53 54 55 56 57 62 63 64
chain bonds :
4-8 8-9 9-17 21-23 23-24 24-25 24-26 26-32 27-28 32-33 33-34
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 40-41 40-45 41-42 42-43 43-44 44-45 47-48 47-51 48-49 49-50 50-51 53-54 53-57 54-55 55-56 56-57 62-63 62-64 63-64
exact/norm bonds :
4-8 8-9 9-17 21-23 23-24 24-25 24-26 26-32 27-28 32-33 33-34 47-48 47-51 48-49 49-50 50-51 53-54 53-57 54-55 55-56 56-57 62-63 62-64 63-64
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 40-41 40-45 41-42 42-43 43-44 44-45
isolated ring systems :
containing 1 : 40 : 47 : 53 :

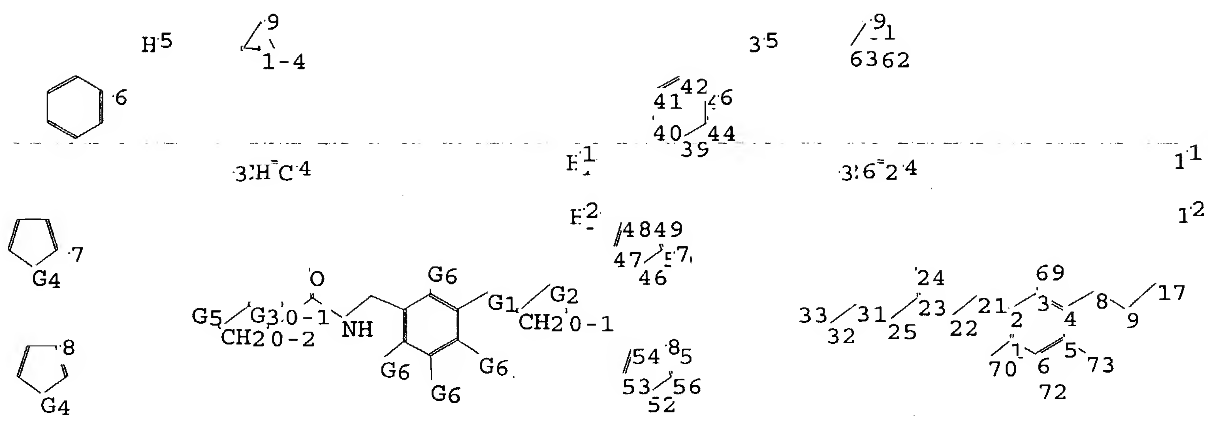
G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]

```
G4:O,S

G5:[*5],[*6],[*7],[*8],[*9]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:Atom  11:Atom
17:CLASS  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS
28:CLASS  32:CLASS  33:CLASS  34:Atom  39:Atom  40:Atom  41:Atom  42:Atom  43:Atom
44:Atom  45:Atom  47:Atom  48:Atom  49:Atom  50:Atom  51:Atom  53:Atom  54:Atom
55:Atom  56:Atom  57:Atom  62:Atom  63:Atom  64:Atom
Generic attributes :
10:
Saturation              : Unsaturated
Number of Carbon Atoms  : less than 7
Number of Hetero Atoms  : less than 2
Type of Ring System     : Monocyclic
11:
Saturation              : Unsaturated
Number of Carbon Atoms  : less than 7
Number of Hetero Atoms  : 2 or more
Type of Ring System     : Monocyclic
39:
Saturation              : Unsaturated
Number of Hetero Atoms  : less than 2

Element Count :
Node 10: Limited
    C,C5
    N,N1
    S,S0
    O,O0

Node 11: Limited
    C,C4
    N,N2
    O,O0
    S,S0

Node 39: Limited
    C,C5-9
    N,N1
    O,O0
    S,S0




L5      STRUCTURE UPLOADED

=> que L5 AND L3 NOT L4

L6   QUE L5 AND L3 NOT L4

=> d 16
L6 HAS NO ANSWERS
L3              SCR 1840
L4              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L5              STR
```

```
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L6              QUE  L5 AND L3 NOT L4

=> s l6 sss sam
SAMPLE SEARCH INITIATED 18:53:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  80732 TO ITERATE

  1.2% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0

L7            0 SEA SSS SAM L5 AND L3 NOT L4

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1840

L8    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L9    SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538 (b).str
```



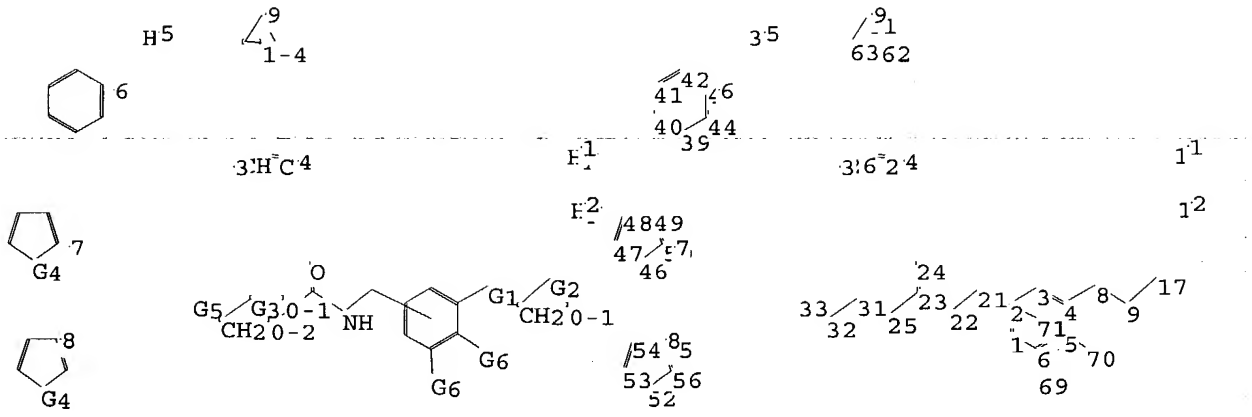
chain nodes :
8 9 10 11 17 21 22 23 24 25 26 27 31 32 33 38 69 70 72 73
ring nodes :
1 2 3 4 5 6 39 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56
61 62 63
chain bonds :
1-70 2-21 3-69 4-8 5-73 6-72 8-9 9-17 21-22 22-23 23-24 23-25 25-31
26-27 31-32 32-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-44 40-41 41-42 42-43 43-44 46-47
46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55 55-56 61-62 61-63 62-63
exact/norm bonds :
1-70 2-21 3-69 4-8 5-73 6-72 8-9 9-17 21-22 22-23 23-24 23-25 25-31
26-27 31-32 32-33 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
55-56 61-62 61-63 62-63
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-44 40-41 41-42 42-43 43-44
isolated ring systems :
containing 1 : 39 : 46 : 52 :

G1:O,N

G2:[*1],[*2]

```
G3:CH2,[*3-*4]

G4:O,S

G5:[*5],[*6],[*7],[*8],[*9]

G6:H,Cl,Br,F,I

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:Atom  11:Atom
17:CLASS  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS
31:CLASS  32:CLASS  33:Atom  38:Atom  39:Atom  40:Atom  41:Atom  42:Atom  43:Atom
44:Atom  46:Atom  47:Atom  48:Atom  49:Atom  50:Atom  52:Atom  53:Atom  54:Atom
55:Atom  56:Atom  61:Atom  62:Atom  63:Atom  69:CLASS  70:CLASS  72:CLASS  73:CLASS

Generic attributes :
10:
Saturation              : Unsaturated
Number of Carbon Atoms  : less than 7
Number of Hetero Atoms  : less than 2
Type of Ring System     : Monocyclic
11:
Saturation              : Unsaturated
Number of Carbon Atoms  : less than 7
Number of Hetero Atoms  : 2 or more
Type of Ring System     : Monocyclic
38:
Saturation              : Unsaturated
Number of Hetero Atoms  : less than 2

Element Count :
Node 10: Limited
    C,C5
    N,N1
    S,S0
    O,O0

Node 11: Limited
    C,C4
    N,N2
    O,O0
    S,S0

Node 38: Limited
    C,C5-9
    N,N1
    O,O0
    S,S0




L10     STRUCTURE UPLOADED

=> que L10 AND L8 NOT L9

L11  QUE L10 AND L8 NOT L9
```

```
=> d l11
L11 HAS NO ANSWERS
L8              SCR 1840
L9              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L10             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L11             QUE  L10 AND L8 NOT L9


=> s l11 sss sam
SAMPLE SEARCH INITIATED 18:55:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   2266 TO ITERATE

 44.1% PROCESSED    1000 ITERATIONS                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        42465 TO    48175
PROJECTED ANSWERS:               0 TO        0

L12           0 SEA SSS SAM L10 AND L8 NOT L9

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1840

L13   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L14   SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538 (d).str
```



chain nodes :
8 9 10 11 17 21 22 23 24 25 26 27 31 32 33 38 69 70
ring nodes :
1 2 3 4 5 6 39 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56
61 62 63
chain bonds :
4-8 5-70 6-69 8-9 9-17 21-22 22-23 23-24 23-25 25-31 26-27 31-32 32-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-44 40-41 41-42 42-43 43-44 46-47
46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55 55-56 61-62 61-63 62-63
exact/norm bonds :
4-8 5-70 6-69 8-9 9-17 21-22 22-23 23-24 23-25 25-31 26-27 31-32 32-33
46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55 55-56 61-62 61-63
62-63
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-44 40-41 41-42 42-43 43-44
isolated ring systems :
containing 1 : 39 : 46 : 52 :

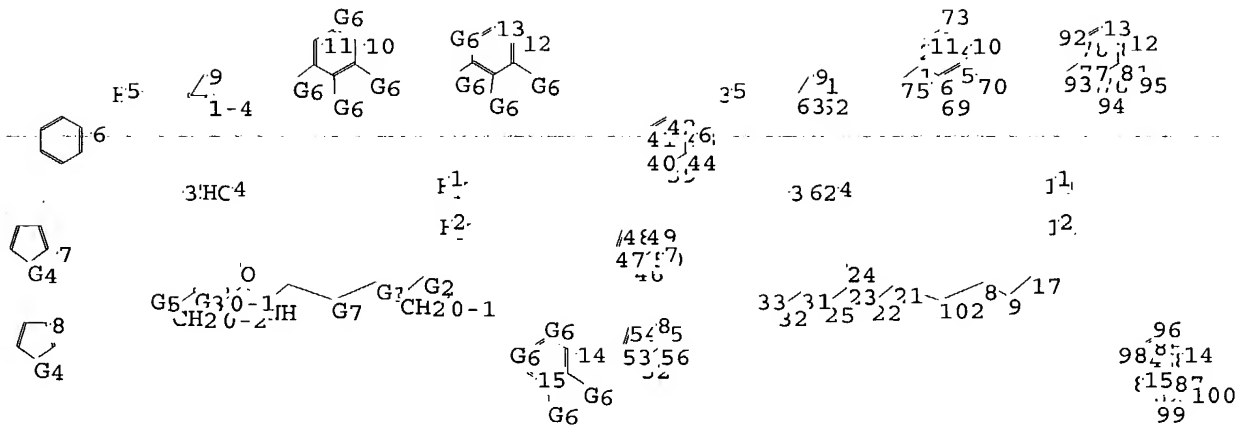
G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]

```
G4:O,S

G5:[*5],[*6],[*7],[*8],[*9]

G6:H,Cl,Br,F,I

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:Atom  11:Atom
17:CLASS  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS
31:CLASS  32:CLASS  33:Atom  38:Atom  39:Atom  40:Atom  41:Atom  42:Atom  43:Atom
44:Atom  46:Atom  47:Atom  48:Atom  49:Atom  50:Atom  52:Atom  53:Atom  54:Atom
55:Atom  56:Atom  61:Atom  62:Atom  63:Atom  69:CLASS  70:CLASS  71:CLASS
Generic attributes :
10:
Saturation              : Unsaturated
Number of Carbon Atoms  : less than 7
Number of Hetero Atoms  : less than 2
Type of Ring System     : Monocyclic
11:
Saturation              : Unsaturated
Number of Carbon Atoms  : less than 7
Number of Hetero Atoms  : 2 or more
Type of Ring System     : Monocyclic
38:
Saturation              : Unsaturated
Number of Hetero Atoms  : less than 2

Element Count :
Node 10: Limited
    C,C5
    N,N1
    S,S0
    O,O0

Node 11: Limited
    C,C4
    N,N2
    O,O0
    S,S0

Node 38: Limited
    C,C5-9
    N,N1
    O,O0
    S,S0




L15     STRUCTURE UPLOADED

=> que L15 AND L13 NOT L14

L16  QUE L15 AND L13 NOT L14

=> d l16
L16 HAS NO ANSWERS
```

```
L13             SCR 1840
L14             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L15             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *
Structure attributes must be viewed using STN Express query preparation.
L16             QUE  L15 AND L13 NOT L14


=> s l16 sss sam
SAMPLE SEARCH INITIATED 18:57:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  80732 TO ITERATE

  1.2% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0

L17           0 SEA SSS SAM L15 AND L13 NOT L14

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1840

L18   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L19   SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538 (e).str
```



chain nodes :
8 9 10 11 17 21 22 23 24 25 26 27 31 32 33 38 69 70 73 75 92
93 94 95 96 98 99 100 102
ring nodes :
1 2 3 4 5 6 39 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56
61 62 63 76 77 78 79 80 81 82 83 84 85 86 87
chain bonds :
1-75 3-73 5-70 6-69 8-9 8-102 9-17 21-22 21-102 22-23 23-24 23-25 25-31
26-27 31-32 32-33 76-94 77-93 78-92 81-95 82-99 84-98 85-96 87-100
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-44 40-41 41-42 42-43 43-44 46-47
46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55 55-56 61-62 61-63 62-63
76-77 76-81 77-78 78-79 79-80 80-81 82-83 82-87 83-84 84-85 85-86 86-87
exact/norm bonds :
1-75 3-73 5-70 6-69 8-9 8-102 9-17 21-22 21-102 22-23 23-24 23-25 25-31
26-27 31-32 32-33 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
55-56 61-62 61-63 62-63 76-94 77-93 78-92 81-95 82-99 84-98 85-96
87-100
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-44 40-41 41-42 42-43 43-44 76-77
76-81 77-78 78-79 79-80 80-81 82-83 82-87 83-84 84-85 85-86 86-87
isolated ring systems :
containing 1 : 39 : 46 : 52 : 76 : 82 :

```
G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]

G4:O,S

G5:[*5],[*6],[*7],[*8],[*9]

G6:H,Cl,Br,F,I

G7:[*10-*11],[*12-*13],[*14-*15]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:Atom  11:Atom
17:CLASS  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS
31:CLASS  32:CLASS  33:Atom  38:Atom  39:Atom  40:Atom  41:Atom  42:Atom  43:Atom
44:Atom  46:Atom  47:Atom  48:Atom  49:Atom  50:Atom  52:Atom  53:Atom  54:Atom
55:Atom  56:Atom  61:Atom  62:Atom  63:Atom  69:CLASS  70:CLASS  73:CLASS  75:CLASS
 76:Atom  77:Atom  78:Atom  79:Atom  80:Atom  81:Atom  82:Atom  83:Atom  84:Atom
85:Atom  86:Atom  87:Atom  92:CLASS  93:CLASS  94:CLASS  95:CLASS  96:CLASS
98:CLASS  99:CLASS  100:CLASS  102:CLASS
Generic attributes :
10:
Saturation              : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System     : Monocyclic
11:
Saturation              : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System     : Monocyclic
38:
Saturation              : Unsaturated
Number of Hetero Atoms : less than 2

Element Count :
Node 10: Limited
    C,C5
    N,N1
    S,S0
    O,O0

Node 11: Limited
    C,C4
    N,N2
    O,O0
    S,S0

Node 38: Limited
    C,C5-9
    N,N1
    O,O0
    S,S0
```

```
L20     STRUCTURE UPLOADED
=> que L20 AND L18 NOT L19

L21  QUE L20 AND L18 NOT L19

=> d l21
L21 HAS NO ANSWERS
L18             SCR 1840
L19             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L20             STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L21             QUE  L20 AND L18 NOT L19


=> s l21 sss sam
SAMPLE SEARCH INITIATED 19:01:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  16543 TO ITERATE

  6.0% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       323163 TO   338557
PROJECTED ANSWERS:               0 TO        0

L22           0 SEA SSS SAM L20 AND L18 NOT L19

=> s l21 sss ful
FULL SEARCH INITIATED 19:01:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 330291 TO ITERATE

100.0% PROCESSED  330291 ITERATIONS                              7 ANSWERS
SEARCH TIME: 00.00.09

L23           7 SEA SSS FUL L20 AND L18 NOT L19

=> => s l23
L24           2 L23

=> d l24 1-2 bib,ab,hitstr
```

L24 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:268482 CAPLUS
DN 128:321930
TI Preparation of β-thiopropionylamino acid derivatives as β-lactamase inhibitors
IN Bateson, John Hargreaves; Best, Desmond John; Clarke, Brian Peter; Gilpin, Martin Leonard; Witty, David R.; et al.
PA Smithkline Beecham Plc, UK; Bateson, John Hargreaves; Best, Desmond John; Clarke, Brian Peter; Gilpin, Martin Leonard
SO PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9817639	A1	19980430	WO 1997-EP5709	19971010
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9850501	A1	19980515	AU 1998-50501	19971010
	EP 934262	A1	19990811	EP 1997-913147	19971010
	R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
	JP 2001502345	T2	20010220	JP 1998-518931	19971010
	US 6156774	A	20001205	US 1999-284098	19990407
PRAI	GB 1996-21692	A	19961017		
	GB 1997-4581	A	19970305		
	GB 1997-16212	A	19970731		
	WO 1997-EP5709	W	19971010		

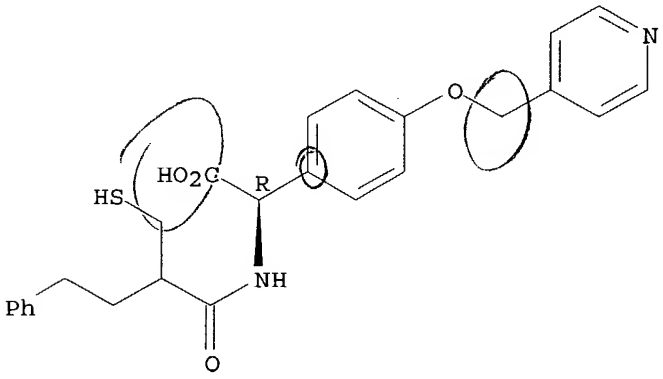
OS MARPAT 128:321930
AB Title mercapto amino acid derivs. R4SCR5R6CHR3CONR2CHR1CO2R [I; R = H, salt-forming cation of in vivo hydrolyzable ester-forming group; R1 = Q, Q1; ring A = monocyclic aryl or heteroaryl ring; ring B = monocyclic aryl, alicyclic, or heterocyclic ring; C, D = Zp(CR8CR9)q, (CR8CR9)qZp; p = 0, 1, q = 0-3 provided that p + q ≠ 0 in C; R8, R9 = H, (C1-6)alkyl; CR8R9 = O; Z = O, NR10, S(O)x; R10 = H, (C1-6)alkyl. aryl(C1-6)alkyl; x = 0-2; wherein C and D are linked ortho to one another on each of the rings A and B in Q1; R2 = H, (C1-6)alkyl, aryl(C1-6)alkyl; R3 = H, (C1-6)alkyl substituted by 0-3 halo atoms, (C3-7)cycloalkyl, fused aryl(C3-7)cycloalkyl, (C3-7)cycloalkyl(C2-6)alkyl, (C2-6)alkenyl, (C2-6)alkynyl, aryl, aryl-(CH2)m-X-(CH2)n, heterocyclyl, heterocyclyl-(CH2)m-X-(CH2)n; m = 0-3; n = 1-3; X = O, S(O)x, bond; R4 = H or in vivo hydrolyzable acyl; R5, R6 = H, (C1-6)alkyl; R5R6 = (CH2)2-5] for use in treatment of bacterial infections in humans or animals by administration in combination with a β-lactam antibiotic. Thus, lithiation of thiophene and alkylation with 3-(bromomethyl)tetrahydrofuran gave 2-(tetrahydrofuran-3-ylmethyl)thiophene, which underwent lithiation and acylation with Et oxalyl chloride to give oxoacetate II (X1 = O). II (X1 = O) was converted into hydroxyiminoacetate II (X1 = NOH), reduced in situ to the corresponding amine, acylated with 2-(acetylthio)4-phenylbutanoic acid (preparation given), and saponified to give desired title compound III. III and related mercaptopropionyl derivs. inhibited Bacteroides fragilis CfiA metallo-β-lactamase with IC50 <1 μM. Compound III inhibited Bacteroides fragilis 262 strain, which produces CfiA metallo-β-lactamase, alone with MIC >256 μg/mL, but with MIC 16

μg/mL in the presence of 8 μg/mL meropenem.

IT **206765-11-9P 206765-12-0P 206765-13-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of β-thiopropionylamino acid derivs. as β-lactamase inhibitors)

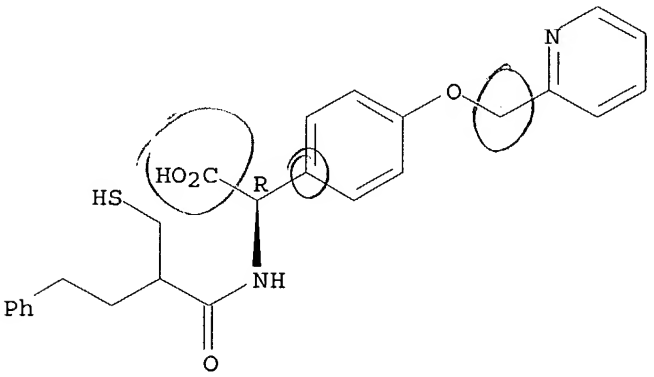
RN 206765-11-9 CAPLUS
CN Benzeneacetic acid, α-[[2-(mercaptomethyl)-1-oxo-4-phenylbutyl]amino]-4-(4-pyridinylmethoxy)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



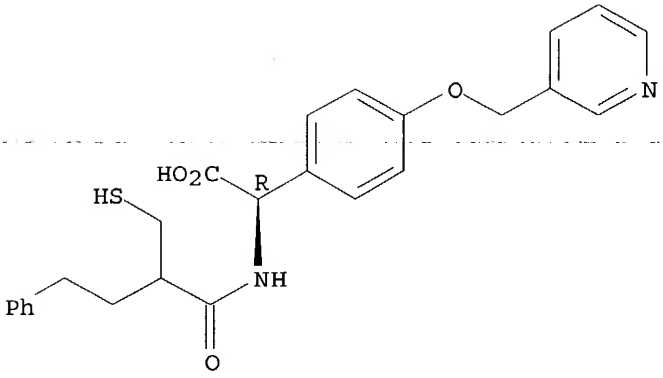
RN 206765-12-0 CAPLUS
CN Benzeneacetic acid, α-[[2-(mercaptomethyl)-1-oxo-4-phenylbutyl]amino]-4-(2-pyridinylmethoxy)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 206765-13-1 CAPLUS
CN Benzeneacetic acid, α-[[2-(mercaptomethyl)-1-oxo-4-phenylbutyl]amino]-4-(3-pyridinylmethoxy)-, (αR)- (9CI) (CA INDEX NAME)

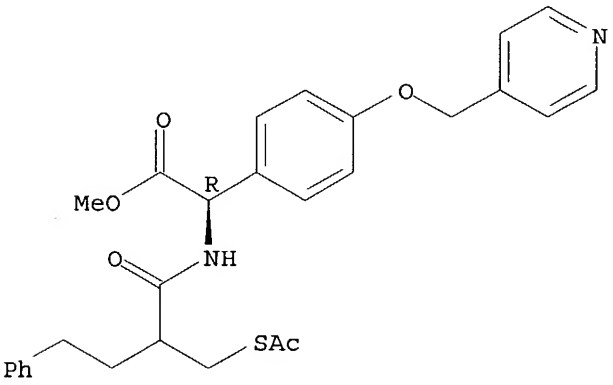
Absolute stereochemistry.



IT **206766-05-4P 206766-06-5P 206766-07-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of β-thiopropionylamino acid derivs. as β-lactamase inhibitors)

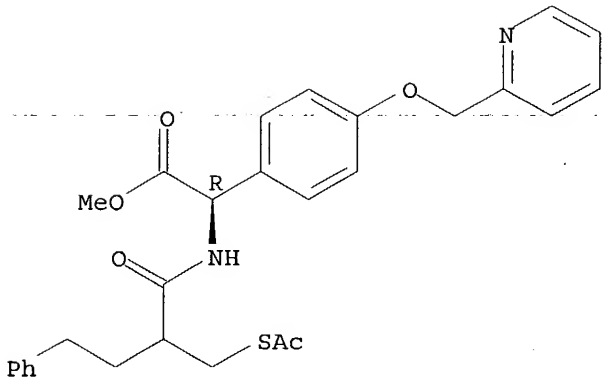
RN 206766-05-4 CAPLUS
CN Benzeneacetic acid, α-[[2-[(acetylthio)methyl]-1-oxo-4-phenylbutyl]amino]-4-(4-pyridinylmethoxy)-, methyl ester, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



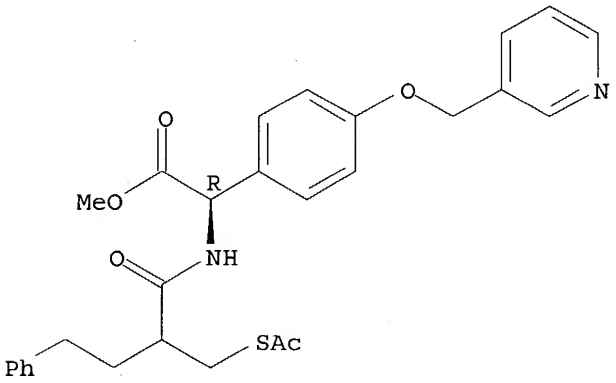
RN 206766-06-5 CAPLUS
CN Benzeneacetic acid, α-[[2-[(acetylthio)methyl]-1-oxo-4-phenylbutyl]amino]-4-(2-pyridinylmethoxy)-, methyl ester, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 206766-07-6 CAPLUS
CN Benzeneacetic acid, α-[[2-[(acetylthio)methyl]-1-oxo-4-phenylbutyl]amino]-4-(3-pyridinylmethoxy)-, methyl ester, (αR)-(9CI) (CA INDEX NAME)

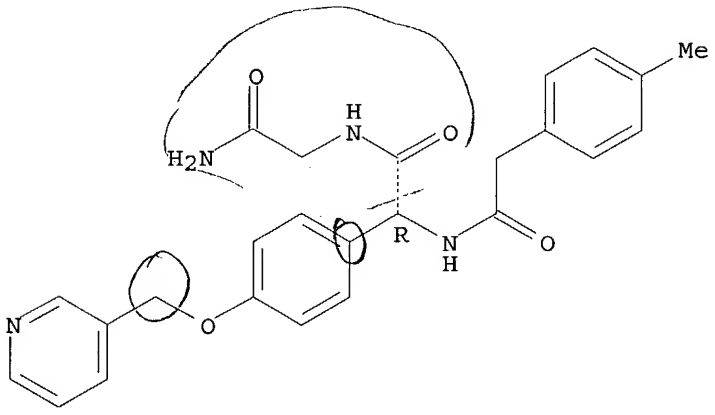
Absolute stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:271992 CAPLUS
DN 125:59045
TI Multipin solid phase synthesis of ethers using modified Mitsunobu chemistry
AU Valerio, Robert M.; Bray, Andrew M.; Patsiouras, Heather
CS Chiron Mimotypes Pty. Ltd., Clayton, 3169, Australia
SO Tetrahedron Letters (1996), 37(17), 3019-22
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
AB Formation of ether derivs. of phenolic containing structures using solid phase Mitsunobu chemical on functionalized polyethylene pins was investigated. Using the multipin approach, a range of reaction parameters were systematically varied in parallel expts. including solvent, temperature, time, reactant concns., base, phosphine and alc. to determine optimum reaction conditions. Solid phase reaction of three phenols with a range of alcs. to form the ethers proceeds smoothly using 0.15M PPh3/DEAD/alc. in THF at 37° for 4 days in the presence of 0.45M Et3N.
IT **178119-96-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(multipin solid phase synthesis of aryl ethers using modified Mitsunobu chemical)
RN 178119-96-5 CAPLUS
CN Glycinamide, N-[(4-methylphenyl)acetyl]-D-2-[4-(3-pyridinylmethoxy)phenyl]glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```
=> => d his

     (FILE 'HOME' ENTERED AT 18:47:07 ON 08 APR 2004)

     FILE 'REGISTRY' ENTERED AT 18:47:12 ON 08 APR 2004
L1                STRUCTURE UPLOADED
L2              0 S L1 SSS SAM
L3                SCREEN 1840
L4                SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L5                STRUCTURE UPLOADED
L6                QUE L5 AND L3 NOT L4
L7              0 S L6 SSS SAM
L8                SCREEN 1840
L9                SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L10               STRUCTURE UPLOADED
L11               QUE L10 AND L8 NOT L9
L12             0 S L11 SSS SAM
L13               SCREEN 1840
L14               SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L15               STRUCTURE UPLOADED
L16               QUE L15 AND L13 NOT L14
L17             0 S L16 SSS SAM
L18               SCREEN 1840
L19               SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L20               STRUCTURE UPLOADED
L21               QUE L20 AND L18 NOT L19
L22             0 S L21 SSS SAM
L23             7 S L21 SSS FUL

     FILE 'CAPLUS' ENTERED AT 19:01:54 ON 08 APR 2004
L24             2 S L23

     FILE 'CAOLD' ENTERED AT 19:02:16 ON 08 APR 2004

=> s l23
L25           0 L23

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.42     176.08

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -1.39

STN INTERNATIONAL LOGOFF AT 19:02:28 ON 08 APR 2004
```